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13. ABSTRACT *(Maximum 200 words)*
This project focused on the numerical algorithms and analysis which are needed for the effective real-time simulation of mechanical systems. Real-time simulation of mechanical systems is needed in robotics, as well as in the design and simulation of vehicles, including automobiles, high-speed trains, tanks and construction equipment. A number of related projects were proposed which would enable improved capabilities for real-time simulation of systems from mechanics, and also of related electrical, chemical and power systems. Proposed research included analysis and numerical algorithm development addressing these issues: problem formulation and numerical stability, exploiting structure and parallelism, high-frequency oscillations, rank-deficient constraints, discontinuities and delays.

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NUMERICAL METHODS FOR DIFFERENTIAL-ALGEBRAIC EQUATIONS IN REAL-TIME INTEGRATION OF MECHANICAL SYSTEMS

FINAL PROGRESS REPORT

LINDA R. PETZOLD

MARCH 15, 1996

U.S. ARMY RESEARCH OFFICE

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UNIVERSITY OF MINNESOTA

1 Statement of the problem studied

This project focused on the numerical algorithms and analysis which are needed for the effective real-time simulation of mechanical systems. Real-time simulation of mechanical systems is needed in robotics, as well as in the design and simulation of vehicles, including automobiles, high-speed trains, tanks and construction equipment. A number of related projects were proposed which would enable improved capabilities for real-time simulation of systems from mechanics, and also of related electrical, chemical and power systems. Proposed research included analysis and numerical algorithm development addressing these issues: problem formulation and numerical stability, exploiting structure and parallelism, high-frequency oscillations, rank-deficient constraints, discontinuities and delays.

2 Summary of the most important results

High-frequency oscillations in an ODE/DAE are a problem in vehicle simulation because following the oscillations necessitates the use of an extremely small timestep. However, many of the oscillations are not important for the overall numerical solution. Experiments have shown that certain implicit methods combined with automatic stepsize control can damp out the oscillation safely, in regions where its amplitude is too small to be important. There is also some theory to support this technique for the equations of motion. However, once the stepsize is increased, problems with Newton iteration convergence again restrict the timestep. Some formulations of the equations of motion are more advantageous than others in terms of Newton iteration convergence for highly oscillatory systems. A coordinate-split (CS) method has been developed that, together with a modified Newton (CM) iteration is particularly effective. Numerical results for a bushing problem demonstrate that the new method is particularly effective for highly oscillatory systems where the oscillation is small and can be damped. Recently developed theory explains the Newton convergence results. Investigation of the high-frequency oscillation problem was motivated by discussions with Roger Wehage and Jim Overholt (TARDEC).

Significant new software packages have been developed. Data-parallel and message-passing versions of DASPK, which combines the time-stepping methods of our DAE solver DASSL with the preconditioned iterative method GMRES for solving the linear systems at each Newton iteration, were completed. A method for finding consistent initial conditions for several large classes of DAEs was developed in collaboration with A. C. Hindmarsh and P. N. Brown of LLNL. The new method is particularly effective when used in conjunction with DASSL/DASPK because it uses the same iteration matrix/preconditioner as DASSL/DASPK. Codes based on DASSL and DASPK which offer sensitivity analysis have been developed, along with some new algorithms and theory.

Differential-algebraic systems with rank-deficient constraints pose problems for numerical methods. There are many kinds of singularities which can occur. Some lead to bifurcations or impasse points; others are kinematic singularities where the solution is well-defined through the singularity. Regularizations have been developed for index-one and for Hessenberg index-two systems such as multibody systems for dealing with kinematic singularities. Theory has been developed in the linear case to show that the solution to the regularized system is well-defined through the singularity and converges to the true solution as the regularization parameter $\epsilon \to 0$. The methods are motivated by trust region methods in numerical optimization. Tests on a singular slider-crank mechanism show that the methods are robust and relatively easy to implement. This work has been done in collaboration with Y. Ren (University of Bath) and Peter Moore (Tulane University).

Numerical methods have been developed for delay-differential-algebraic equations of retarded and neutral type. These types of equations arise in real-time simulation, where time delays can be introduced by the computer time needed to compute an output after the input has been sampled, and where additional delays can be introduced by the operator-in-the-loop. Delays arise also in circuit simulation and power systems, due for example to interconnects for computer chips and transmission lines, and in chemical process simulation when modeling pipe flow. Convergence results for linear multistep and Runge-Kutta methods applied to delay differential-algebraic equations (DDAEs) of index 1 and 2, retarded or neutral types were developed. This work was done in collaboration with Prof. U. Ascher (University of British

Columbia).

3 Publications and Technical Reports

P. K. Moore, L. R. Petzold and Y. Ren, *Regularization of Index-One Differential-Algebraic Equations with Rank-Deficient Constraints*, submitted to Mathematics of Computation.

L. R. Petzold and J. Yen, *An Efficient Newton-Type Iteration for the Numerical Solution of Highly Oscillatory Constrained Multibody Dynamic Systems*, submitted to SIAM J. Sci. Comput.

P. N. Brown, A. C. Hindmarsh and L. R. Petzold, *Consistent Initial Condition Calculation for Differential-Algebraic Systems*, submitted to SIAM J. Sci. Comput.

T. Maly and L. R. Petzold, *Numerical Methods and Software for Sensitivity Analysis of Differential-Algebraic Systems*, to appear, Applied Numerical Mathematics.

L. R. Petzold and A. C. Hindmarsh, *Algorithms and Software for Ordinary Differential Equations and Differential-Algebraic Equations*, Part I and Part II, Computers in Physics, 1995.

R. S. Maier, L. R. Petzold and W. Rath, *Parallel Solution of Large-Scale Differential-Algebraic Systems*, Concurrency: Practice and Experience 7, 795-822, 1995.

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A. C. Hindmarsh, P. N. Brown and L. R. Petzold, *Using Krylov Methods in the Solution of Large-Scale Differential-Algebraic Systems*, to appear, SIAM J. Scientific Computing.

U. Ascher and L. R. Petzold, *The Numerical Solution of Delay-Differential-Algebraic Equations of Retarded and Neutral Type*, SIAM J. on Numerical Analysis 32, (1995), 1635-1657.

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J. Yen and L. R. Petzold, *Numerical Solution of Nonlinear Oscillatory Multibody Systems*, to appear, Proc. Dundee Numerical Analysis Conference, 1995.

L. O. Jay and L. R. Petzold, *Highly Oscillatory Systems and Periodic-Stability*, Dept. of Computer Science, University of Minnesota, 1995.

J. Yen and L. R. Petzold, *On the Numerical Solution of Constrained Multibody Dynamic Systems*, Dept. of Computer Science, University of Minnesota, 1994.

J. Yen and L. R. Petzold, *Computational Challenges in the Solution of Nonlinear Highly Oscillatory Multibody Systems*, in Numerical Analysis of Ordinary Differential Equations and its Applications, ed. T. Mitsui and Y.

Shinohara, World Scientific, 1995.

4 List of all participating scientific personnel

The personnel participating in this project were: PI: Linda R. Petzold, Graduate Research Assistants: Werner Rath, Rongze Zhao, Cecil Smith, Wenjie Zhu, Shengtai Li. Rongze Zhao earned a Ph.D. in Aerospace Engineering while employed by the project.

5 Report of inventions

None.